An optimization procedure to estimate the dielectric constant of solid materials

Hyperspectral Advanced R&D for Solids (PL14-FY14-112-PD3WA)

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Abstract

Dispersive analysis can be used to give a material's optical properties, such as complex index of refraction as measured by n and k, both functions of frequency. We use dispersive analysis to yield the effective dielectric constant of a solid material given its reflectance spectrum, assuming Lorentz lines comprise a significant portion of the observed reflectance. Lorentz lines are simple resonances in the near-normal reflectance spectrum that do not interact with one another. For the purpose of assisting hyperspectral imaging technologies, we developed an optimization procedure to fit Lorentz line resonances to an observed reflectance in the long-wave infrared spectrum. We use a stepwise optimization algorithm to estimate the material's effective dielectric constant—a complex valued function of frequency—through placement of oscillators in the Lorentz line formula. We demonstrate the effectiveness of this fitting procedure using laboratory reflectance measurement for calcite of various particle sizes. Adequate recovery of the dielectric constant given reflectance may lead to improvements in the detection of specific materials.

Goals and Objectives

- Improved estimation of effective dielectric constant
- Fully automated fitting method given reflectance spectrum
- Fit oscillators of material via Drude-Lorentz formula
- Balance adequate reflectance fitting with overfitting

Optical Properties of Solid Materials

Optical quantities are all functions of a complex-valued dielectric constant, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$, as a function of frequency.

Dispersion theory yields the optical properties n and k from near-normal reflectance spectrum R(ω).

Assume this reflectance spectrum consists of non-interacting oscillators (Lorentz lines or optical resonances).

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = \varepsilon_\infty + \sum_{j=1}^{p} \frac{A_j \omega_{Oj}^2}{\omega_{Oj}^2 - \omega^2 - i\gamma_j \omega}$$

From the dielectric constant, the optimal properties $n(\omega)$ and $k(\omega)$ are calculated along with the reflectance R(ω) at normal incidence:

$$N(\omega) = n(\omega) + ik(\omega) = \sqrt{\varepsilon(\omega)}$$

$$R(\omega) = \left| \frac{1 - N(\omega)}{1 + N(\omega)} \right|^2$$

Current Software: RefFIT

RefFIT freeware dielectric fitting tool by A.B. Kuzmenko available at http://optics.unige.ch/alexey/reffit.html

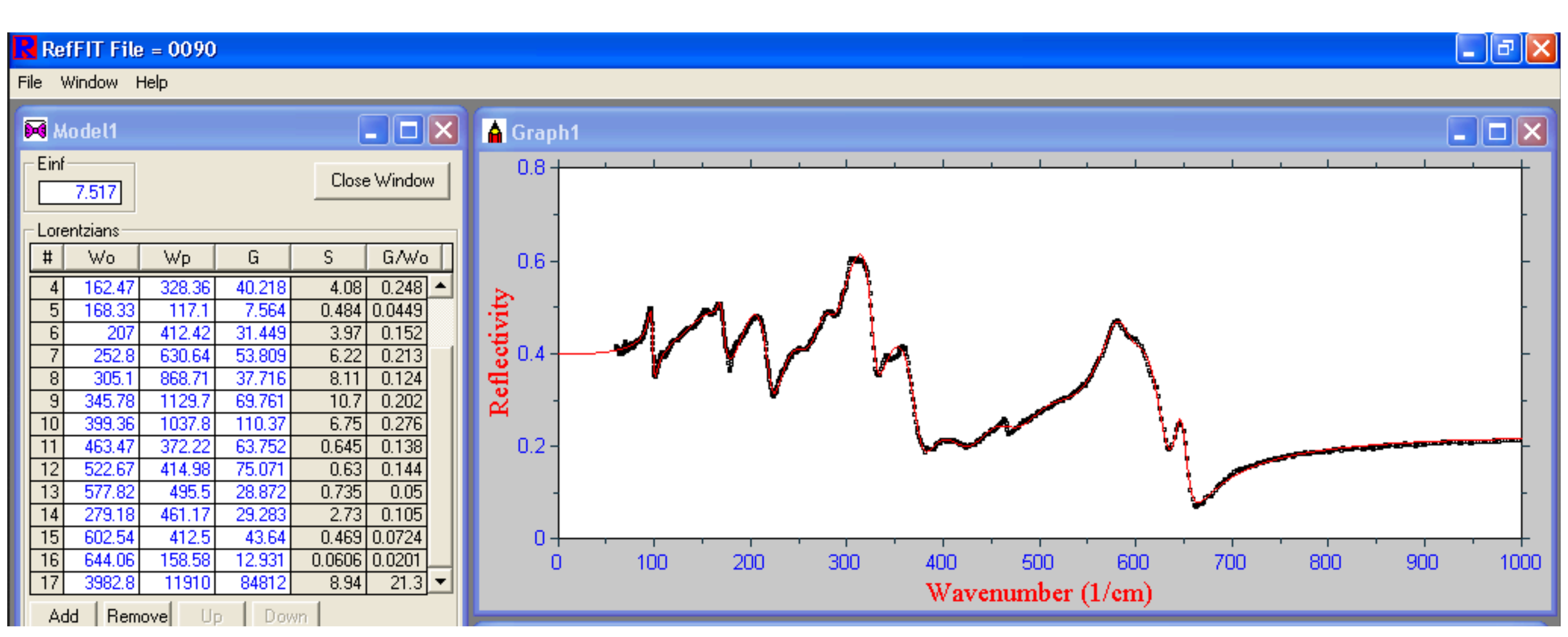


Figure: Screenshot of RefFIT program (from website).

- Uses Drude-Lorentz oscillators formula for fitting (W_O, W_P, G)
- Calculates optimal values for all 3p+1 fit parameters

Deficiencies:

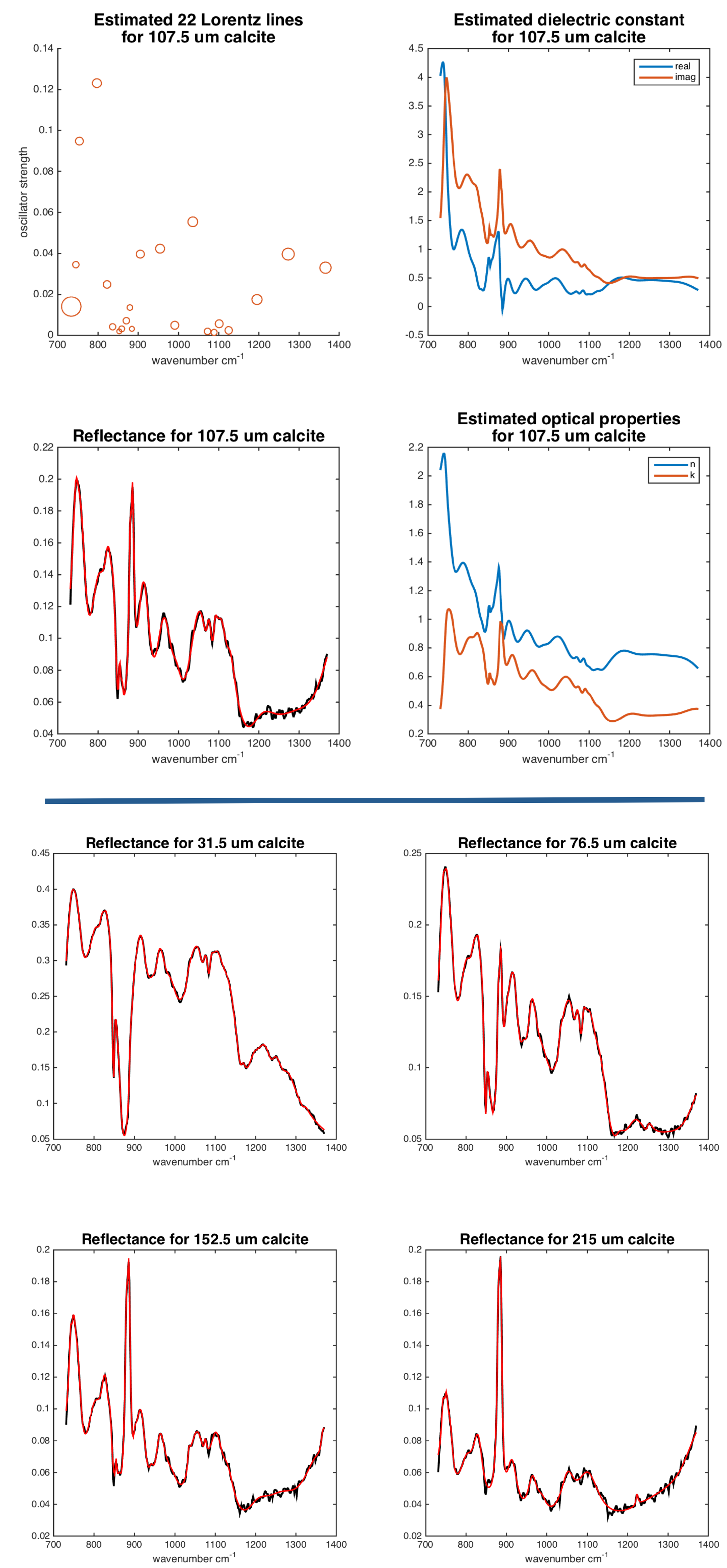
- not automated
- have to provide guesses for oscillator frequencies
- if guesses are not close then fits are poor

Fitting Procedure

- Forward stepwise procedure, adding resonances
- Minimizes squared residuals, Levenberg-Marquardt optimization
- Two stage search per step, second stage can be skipped if significant improvement found in first stage
- Parameters held constant for oscillators far from proposed frequency—reducing optimization parameters, increasing speed
- R^2-adjusted stopping rule used to discourage overfitting

Results

Fitting laboratory spectra of calcite particles (Univ. Arizona Astronomy)



References

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